Methylcitric acid, tetraTBDMS (2)

Inchi: InChI=1S/C31H66O7Si4/c1-23(25(33)36-40(16,17)28(5,6)7)31(38-42(20,21)30(11,12)13
InchiKey: RGQSPHREDDNOIS-UHFFFAOYSA-N
Formula: C31H66O7Si4
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)C(CC(=O)O[Si](C)(C)C(C)(C)C)(O[Si](C)(C)C(C)(C)C)C(=
Mol. weight [g/mol]: 663.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.55		Crippen Method
logp	9.418		Crippen Method
rinpol	2692.00		NIST Webbook
rinpol	2692.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R277088&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices